

# Structure of Fermionic Density Matrices: Complete $N$ -representability Conditions

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We present a constructive solution to the  $N$ -representability problem—a full characterization of the conditions for constraining the two-electron reduced density matrix (2-RDM) to represent an  $N$ -electron density matrix. Previously known conditions, while rigorous, were incomplete. Here we derive a hierarchy of constraints built upon (i) the bipolar theorem and (ii) tensor decompositions of model Hamiltonians. Existing conditions  $D$ ,  $Q$ ,  $G$ ,  $T1$ , and  $T2$ , known classical conditions, and new conditions appear naturally. Subsets of the conditions are amenable to polynomial-time computations of strongly correlated systems.

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The wavefunction of a many-electron quantum system contains significantly more information than necessary for the calculation of energies and properties. In 1955 Mayer proposed in *Physical Review* computing the ground-state energy variationally as a functional of the two-electron reduced density matrix (2-RDM) which, unlike the wavefunction, scales polynomially with the number  $N$  of electrons [1–3]. However, the 2-electron density matrix must be constrained to represent a many-electron (or  $N$ -electron) density matrix (or wavefunction); otherwise, the minimized energy is unphysically below the ground-state energy for  $N > 2$ . Coleman called these constraints  *$N$ -representability conditions* [4], and the search for them became known as the  *$N$ -representability problem* [5–10]. In 1995 the National Research Council ranked the  *$N$ -representability problem* as one of the top unsolved theoretical problems in chemical physics [11]. While progress was limited for many years, recent advances in theory and optimization [12–20] have enabled the application of the variational 2-RDM method to studying strong correlation in quantum phase transitions [21], quantum dots [22], polyaromatic hydrocarbons [23], firefly bioluminescence [24], and metal-to-insulator transitions [25].

Despite the recent computational results with 2-RDM methods, a complete set of  *$N$ -representability conditions* on the 2-RDM—not dependent upon higher-order RDMs—has remained unknown. While formal solutions of the  *$N$ -representability problem* were developed in the 1960s [5, 26], practically they required the  *$N$ -electron density matrix* [1, 2]. In this Letter we present a constructive solution of the  *$N$ -representability problem* that generates a complete set of  *$N$ -representability conditions* on the 2-RDM. The approach is applicable to generating the  *$N$ -representability conditions* on the  *$p$ -RDM* for any  $p \leq N$ . The conditions arise naturally as a hierarchy of constraints on the 2-RDM, which we label the  $(2, q)$ -positivity conditions, where the  $(2, 2)$ - and  $(2, 3)$ -positivity conditions include the already known  $D$ ,  $Q$ ,  $G$ ,  $T1$ , and  $T2$  conditions [4, 5, 7, 15]. The second number in  $(2, q)$  corresponds to the higher  $q$ -RDM which serves

as the starting point for the derivation of the condition.

A key advance in extending the  $(2, q)$ -positivity conditions for  $q > 3$  is the use of tensor decompositions in the model Hamiltonians that expose the boundary of the  *$N$ -representable 2-RDM set*. The decompositions allow the terms in the model Hamiltonians to have no more than two-body interactions through the cancelation of all higher 3-to- $q$ -body terms. A second important element is the recognition that when  $q = r$  where  $r$  is the rank of the one-electron basis set the positivity conditions are complete. The hierarchy of conditions can be thought of as a collection of model Hamiltonians [9]. For example, the ‘basic’  $(2, 2)$ -positivity conditions are both necessary and sufficient constraints for computing the ground-state energies of pairing model Hamiltonians [2, 14], often employed in describing long-range order and superconductivity.

Consider a quantum system composed of  $N$  fermions. A matrix is a fermionic *density matrix* if and only if it is: (i) Hermitian, (ii) normalized (fixed trace), (iii) antisymmetric in the exchange of particles, and (iv) positive semidefinite. A matrix is *positive semidefinite* if and only if its eigenvalues are nonnegative. The  *$p$ -particle reduced density matrix* ( *$p$ -RDM*) can be obtained from the  *$N$ -particle density matrix* by integrating over all but the first  $p$  particles

$${}^p D = \binom{N}{p} \int {}^N D d(p+1) \dots dN. \quad (1)$$

The set of  ${}^N D$  is a convex set which we denote as  $P^N$  while the set  ${}^p D$  is a convex set which we denote as  $P_N^p$ , the set of  *$N$ -representable  $p$ -particle density matrices*. A set is *convex* if and only if the convex combination of any two members of the set is also contained in the set

$$w {}^N D_1 + (1 - w) {}^N D_2 \in P^N, \quad (2)$$

where  $0 \leq w \leq 1$ . The integration in Eq. (1) defines a linear mapping from  $P^N$  to  $P_N^p$ , which preserves its convexity.

The energy of a quantum system in a stationary state can be computed from the Hamiltonian traced against

the state's density matrix. For a system of  $N$  fermions we have

$$E = \text{Tr}(\hat{H}^N D). \quad (3)$$

If the Hamiltonian is a  $p$ -body operator, meaning that it has at most  $p$ -particle interactions, then the energy can be written as a functional of only the  $p$ -RDM

$$E = \text{Tr}(\hat{H}^p D). \quad (4)$$

For a system of  $N$  electrons the Hamiltonian generally has at most pairwise interactions, and hence, the energy can be expressed as a linear functional of the 2-RDM. Except when  $N = 2$ , however, minimizing the energy as a functional of a two-electron density matrix  ${}^2D \in P^2$  yields an energy that is much too low. To obtain the correct ground-state energy, we must constrain the two-electron density matrix to be  $N$ -representable, that is  ${}^2D \in P_N^{2*}$ .

Based on the equivalence of the energy expectation values in Eqs. (3) and (4), we can use the set  $P_N^p$  of  $N$ -representable  $p$ -particle density matrices to define a set  $P_N^{p*}$  of  $p$ -particle (Hamiltonian) operators  ${}^p\hat{O}$  that are positive semidefinite in their trace with any  $N$ -particle density matrix

$$P_N^{p*} = \{{}^p\hat{O} | \text{Tr}({}^p\hat{O} {}^pD) \geq 0 \text{ for all } {}^pD \in P_N^p\}. \quad (5)$$

The set  $P_N^{p*}$  is said to be the *polar* (or dual) of the set  $P_N^p$ . Importantly, by the *bipolar theorem* [26, 27], the set  $P_N^{p*}$  also fully defines its polar set  $P_N^p$  as follows

$$P_N^p = \{{}^pD | \text{Tr}({}^p\hat{O} {}^pD) \geq 0 \text{ for all } {}^p\hat{O} \in P_N^{p*}\}. \quad (6)$$

By Eq. (6) we have a complete characterization of the  $N$ -representable  $p$ -RDMs from a knowledge of all operators  ${}^p\hat{O} \in P_N^{p*}$  [26]. This analysis shows formally that there exists a solution to the  $N$ -representability problem [5, 26], but it does not provide a mechanism for characterizing the set  $P_N^{p*}$ .

To characterize  $P_N^{p*}$ , we assume that the  $N$ -fermion quantum system has  $r$  orbitals and hence,  $r - N$  holes. A convex set can be defined by the enumeration of its *extreme elements*, that is the elements (or members) that cannot be expressed by a convex combination of other elements [2, 27]. The definition of  $P_N^{p*}$  in Eq. (5) for  $p \leq N$  can be extended in second quantization to include  $p > N$

$$P_N^{p*} = \{{}^p\hat{O} | \text{Tr}({}^p\hat{O} {}^N D) \geq 0 \text{ for all } {}^N D\} \quad (7)$$

with the  ${}^p\hat{O}$  being polynomials in creation and annihilation operators of degree  $2p$ . Because in second quantization the value of  $N$  is defined in the density matrices  ${}^N D$  rather than in the operators  ${}^p\hat{O}$  [28], the set  $P_N^{p*}$  provides complete  $N$ -representability conditions on the

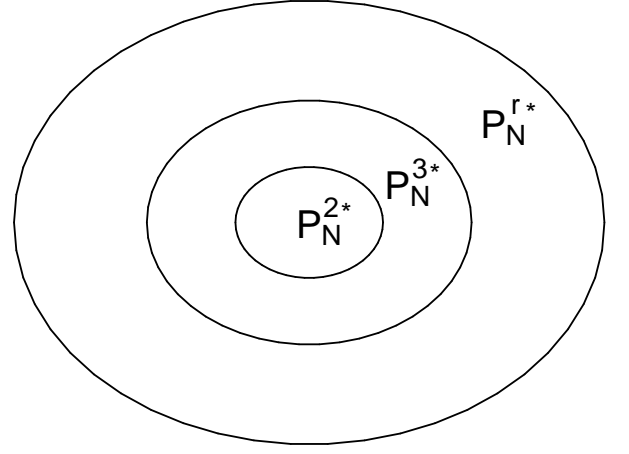


FIG. 1. The convex set  $P_N^{2*}$  of 2-body operators that are positive semidefinite in their trace with any  $N$ -particle density matrix is contained within the convex set  $P_N^{3*}$  of analogous 3-body operators, which in turn is contained within the set  $P_N^{r*}$ . Hence, the extreme points of  $P_N^{2*}$  can be characterized completely by the convex combination of the extreme points of  $P_N^{r*}$ , which are given by Eq. (8).

$p$ -RDM for any  $N$  between 2 and  $r$ . The extreme operators in the set  $P_N^{r*}$  can be written as Hermitian squares of operators [29]

$${}^r\hat{O}_i = {}^r\hat{C}_i {}^r\hat{C}_i^\dagger, \quad (8)$$

where the  ${}^r\hat{C}_i$  are polynomials in the creation and annihilation operators of degree less than or equal to  $r$  (i.e., Eqs. (19) and (20)). Because any operator  ${}^p\hat{C}$  with  $p > r$  reduces to a polynomial of degree  $r$  in its operation on any  ${}^N D$ , the sets  $P_N^{p*}$  with  $p > r$  do not contain additional information about the positivity of  ${}^N D$ . To establish this reduction, we rearrange terms in  ${}^p\hat{C}$  of degree greater than  $r$  into a normal order with either more than  $N$  annihilation operators to the right of the creation operators or more than  $r - N$  creation operators to the right of the annihilation operators; in either situation, the terms of degree greater than  $r$  vanish in their operation upon any  ${}^N D$ .

The operators  ${}^p\hat{O}$  that constrain the  $p$ -RDM to be  $N$ -representable in Eq. (6) are also necessary to constrain the  $q$ -RDM to be  $N$ -representable where  $q > p$ ; formally, each  ${}^p\hat{O} \in P_N^{p*}$  can be lifted by inserting the number operator to the  $(q - p)$  power to form a  ${}^q\hat{O} \in P_N^{q*}$  [14]. Therefore, as illustrated in Fig. 1, we have the following set relations

$$P_N^{2*} \subseteq P_N^{3*} \subseteq P_N^{p*} \dots \subseteq P_N^{r*}. \quad (9)$$

Consequently, extreme operators  ${}^r\hat{O}_i$  of  $P_N^{r*}$  can be combined convexly to produce all  $p$ -body operators  ${}^p\hat{O} \in P_N^{p*}$ , and hence, the extreme points of  $P_N^{p*}$  can be characterized completely by the convex combination of the

extreme points of  $P_N^{r*}$ . More generally, convex combinations of extreme  ${}^q\hat{O}_i \in P_N^{q*}$  generate all  $p$ -body operators  ${}^p\hat{O} \in P_N^{p*}$  for  $p < q$ . Depending upon the order of the creation and annihilation operators in  ${}^r\hat{O}_i$ , the normal-ordered terms will have either positive or negative coefficients. Convex combinations of the  ${}^r\hat{O}_i$  can be chosen to cancel the coefficients of all terms of degree greater than  $p$ . Extreme elements are generated from the minimum number of convex combinations to effect the cancelation. This characterization of the set  $P_N^{p*}$  provides a *constructive solution* of the  $N$ -representability problem for the  $p$ -RDM.

The constructive solution—convex combinations of the operators in Eq. (8)—generates the existing  $N$ -representability conditions as well as new conditions. The  $(1,1)$ -positivity conditions [4] are derivable from the subset of  ${}^r\hat{C}_i$  operators in Eq. (8) of degree 1

$$\hat{C}_D = \sum_j b_j \hat{a}_j^\dagger \quad (10)$$

$$\hat{C}_Q = \sum_j b_j \hat{a}_j. \quad (11)$$

Keeping the trace of the corresponding one-body operators  ${}^1\hat{O}_D$  and  ${}^1\hat{O}_Q$  against the 1-RDM nonnegative for all values of  $b_j$  yields the conditions,  ${}^1D \succeq 0$  and  ${}^1Q \succeq 0$ , where  ${}^1D$  and  ${}^1Q$  are matrix representations of the 1-particle and the 1-hole RDMs and the symbol  $\succeq$  indicates that the matrix is constrained to be positive semidefinite.

Similarly, the  $(2,2)$ -positivity conditions [5] follow from considering the  ${}^r\hat{C}_i$  operators of degree 2 in Eq. (8)

$$\hat{C}_D = \sum_{jk} b_{jk} \hat{a}_j^\dagger \hat{a}_k^\dagger \quad (12)$$

$$\hat{C}_Q = \sum_{jk} b_{jk} \hat{a}_j \hat{a}_k \quad (13)$$

$$\hat{C}_G = \sum_{jk} b_{jk} \hat{a}_j^\dagger \hat{a}_k. \quad (14)$$

Restricting the trace of the corresponding two-body operators  ${}^2\hat{O}_D$ ,  ${}^2\hat{O}_Q$ , and  ${}^2\hat{O}_G$  against the 2-RDM to be nonnegative for all values of  $b_{jk}$  defines the conditions,  ${}^2D \succeq 0$ ,  ${}^2Q \succeq 0$ , and  ${}^2G \succeq 0$ , which constrain the probabilities for finding two particles, two holes, and a particle-hole pair to be nonnegative, respectively.

In general, the  $(q,q)$ -positivity conditions [12, 14] follow from restricting all  $q$ -body operators  ${}^q\hat{O}$  in Eq. (8) to be nonnegative in their trace against the  $q$ -RDM [14]. While the  $(q,q)$ -positive operators are not two-body operators for  $q > 2$ , convex combinations of them generate two-body operators  ${}^2\hat{O} \in P_N^{2*}$  that enforce the  $N$ -representability of the 2-RDM. We refer to necessary  $N$ -representability conditions arising from convex combinations of  $(q,q)$ -positivity conditions as  $(2,q)$ -positivity conditions.

The simplest such constraints, the  $(2,3)$ -positivity conditions, arise from keeping convex combinations of 3-body operators in Eq. (8) nonnegative; for example,

$${}^2\hat{O}_{T1} = \frac{1}{2}(\hat{C}_{T1,1} \hat{C}_{T1,1}^\dagger + \hat{C}_{T1,2} \hat{C}_{T1,2}^\dagger) \quad (15)$$

$${}^2\hat{O}_{T2} = \frac{1}{2}(\hat{C}_{T2,1} \hat{C}_{T2,1}^\dagger + \hat{C}_{T2,2} \hat{C}_{T2,2}^\dagger) \quad (16)$$

where

$$\hat{C}_{T1,1} = \sum_{jkl} b_{jkl} \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l^\dagger \quad (17)$$

$$\hat{C}_{T1,2} = \sum_{jkl} b_{jkl}^* \hat{a}_j \hat{a}_k \hat{a}_l \quad (18)$$

$$\hat{C}_{T2,1} = \sum_{jkl} b_{jkl} \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l + \sum_j b_j \hat{a}_j^\dagger \quad (19)$$

$$\hat{C}_{T2,2} = \sum_{jkl} b_{jkl}^* \hat{a}_j \hat{a}_k \hat{a}_l^\dagger + \sum_j d_j \hat{a}_j. \quad (20)$$

These conditions, known as the  $T1$  and generalized  $T2$  conditions were developed by Erdahl [7] and implemented by Zhao *et al.* [15] and Mazziotti [14]. In general, they significantly improve the accuracy of the 2-positivity conditions.

Although the constructive proof given above indicates that a complete set of  $N$ -representability conditions can be generated from convex combinations of extreme elements of  $P_N^{r*}$ , additional conditions have not been discovered beyond the  $(2,2)$ - and  $(2,3)$ -positivity conditions. For example, what about  $(2,4)$ -positivity conditions—that is,  $N$ -representability constraints on the 2-RDM arising from convex combinations of 4-body operators in Eq. (8)? First, we derive a class of  $(3,4)$ -positivity conditions on the 3-RDM.

Consider the nonnegativity of the following operator  $\hat{O}$  formed by the convex combination of a pair of 4-body operators from Eq. (8)

$$\hat{O} = \frac{1}{2}(\hat{C}_{xxxx} \hat{C}_{xxxx}^\dagger + \hat{C}_{xooo} \hat{C}_{xooo}^\dagger) \quad (21)$$

where the symbols x and o represent creation and annihilation operators, respectively, in the  $\hat{C}$  operators defined as follows

$$\hat{C}_{xxxx} = \sum_{jklm} b_{jklm} \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_m^\dagger \quad (22)$$

$$\hat{C}_{xooo} = \sum_{jklm} d_{jklm} \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \hat{a}_m. \quad (23)$$

Importantly, the expectation value of  $\hat{O}$  with  $d_{jklm} = b_{jklm}$  requires the 4-RDM because the cumulant part  ${}^4\Delta$  of the 4-RDM [1, 30] does not vanish

$$\sum_{jklmpqst} b_{jklm} b_{pqst}^* ({}^4\Delta_{pqst}^{jklm} - {}^4\Delta_{pklm}^{jqst}) \neq 0. \quad (24)$$

TABLE I. A class of (2,4)-positivity conditions can be derived from convex combinations of the (4,4)-positivity conditions that cancel the 3- and 4-particle operators. We achieve the cancelation through tensor decomposition in the model Hamiltonians.

(2,4)-Positivity Conditions	
$\text{Tr}((3\hat{C}_{xxxx}^{\dagger}\hat{C}_{xxxx} + \hat{C}_{xxxo}\hat{C}_{xxxo}^{\dagger} + \hat{C}_{xxox}\hat{C}_{xxox}^{\dagger} + \hat{C}_{xoxx}\hat{C}_{xoxx}^{\dagger} + \hat{C}_{oxxx}\hat{C}_{oxxx}^{\dagger} + \hat{C}_{ooxo}\hat{C}_{ooxo}^{\dagger})^2 D) \geq 0$	
$\text{Tr}((3\hat{C}_{xxxo}^{\dagger}\hat{C}_{xxxo} + \hat{C}_{xxxx}\hat{C}_{xxxx}^{\dagger} + \hat{C}_{xxoo}\hat{C}_{xxoo}^{\dagger} + \hat{C}_{xoxo}\hat{C}_{xoxo}^{\dagger} + \hat{C}_{oxxo}\hat{C}_{oxxo}^{\dagger} + \hat{C}_{ooox}\hat{C}_{ooox}^{\dagger})^2 D) \geq 0$	
$\text{Tr}((3\hat{C}_{xxox}^{\dagger}\hat{C}_{xxox} + \hat{C}_{xxoo}\hat{C}_{xxoo}^{\dagger} + \hat{C}_{xxxx}\hat{C}_{xxxx}^{\dagger} + \hat{C}_{xoox}\hat{C}_{xoox}^{\dagger} + \hat{C}_{oxxo}\hat{C}_{oxxo}^{\dagger} + \hat{C}_{ooox}\hat{C}_{ooox}^{\dagger})^2 D) \geq 0$	
$\text{Tr}((3\hat{C}_{xoxx}^{\dagger}\hat{C}_{xoxx} + \hat{C}_{xoxo}\hat{C}_{xoxo}^{\dagger} + \hat{C}_{xoox}\hat{C}_{xoox}^{\dagger} + \hat{C}_{xxxx}\hat{C}_{xxxx}^{\dagger} + \hat{C}_{oxxx}\hat{C}_{oxxx}^{\dagger} + \hat{C}_{oxoo}\hat{C}_{oxoo}^{\dagger})^2 D) \geq 0$	
$\text{Tr}((3\hat{C}_{oxxx}^{\dagger}\hat{C}_{oxxx} + \hat{C}_{oxxo}\hat{C}_{oxxo}^{\dagger} + \hat{C}_{oxxo}\hat{C}_{oxxo}^{\dagger} + \hat{C}_{oxxx}\hat{C}_{oxxx}^{\dagger} + \hat{C}_{xxxx}\hat{C}_{xxxx}^{\dagger} + \hat{C}_{xooo}\hat{C}_{xooo}^{\dagger})^2 D) \geq 0$	
$\text{Tr}((3\hat{C}_{xxoo}^{\dagger}\hat{C}_{xxoo} + \hat{C}_{xxox}\hat{C}_{xxox}^{\dagger} + \hat{C}_{xxoo}\hat{C}_{xxoo}^{\dagger} + \hat{C}_{xooo}\hat{C}_{xooo}^{\dagger} + \hat{C}_{oxxo}\hat{C}_{oxxo}^{\dagger} + \hat{C}_{ooxx}\hat{C}_{ooxx}^{\dagger})^2 D) \geq 0$	
$\text{Tr}((3\hat{C}_{xoox}^{\dagger}\hat{C}_{xoox} + \hat{C}_{xooo}\hat{C}_{xooo}^{\dagger} + \hat{C}_{xoox}\hat{C}_{xoox}^{\dagger} + \hat{C}_{xxox}\hat{C}_{xxox}^{\dagger} + \hat{C}_{ooxx}\hat{C}_{ooxx}^{\dagger} + \hat{C}_{ooxx}\hat{C}_{ooxx}^{\dagger})^2 D) \geq 0$	
$\text{Tr}((3\hat{C}_{xooo}^{\dagger}\hat{C}_{xooo} + \hat{C}_{xoox}\hat{C}_{xoox}^{\dagger} + \hat{C}_{xooo}\hat{C}_{xooo}^{\dagger} + \hat{C}_{xxxx}\hat{C}_{xxxx}^{\dagger} + \hat{C}_{oxxx}\hat{C}_{oxxx}^{\dagger} + \hat{C}_{oxox}\hat{C}_{oxox}^{\dagger})^2 D) \geq 0$	

To obtain additional  $N$ -representability conditions requires that the dependence of the  $\hat{C}$  operators on the expansion coefficients be *generalized from linear to nonlinear*. Specifically, to obtain 3-RDM conditions beyond the (3,3)-positivity constraints, we must factor the 4-particle expansion coefficients  $b_{jklm}$  and  $d_{jklm}$  into products of 3- and 1-particle coefficients  $b_j b_{klm}$  and  $b_j b_{klm}^*$  which cause the cumulant part of the 4-RDM in  $\langle \Psi | \hat{O} | \Psi \rangle$  to vanish

$$\sum_{jklmpqst} b_j b_{klm} b_p^* b_{qst}^* ({}^4\Delta_{pqst}^{jklm} - {}^4\Delta_{pqst}^{jklm}) = 0. \quad (25)$$

The (3,4)-positivity condition, represented by Eq. (21) and the tensor decomposition of the expansion coefficients, is part of a class of (3,4)-conditions that arises from all distinct combinations of two 4-particle metric matrices that differ from each other in the replacement of *three* second-quantized operators by their adjoints.

A class of (2,4)-positivity conditions, shown in Table I, can be derived from convex combinations of the above (3,4)-positivity conditions that cancel the 3-particle operators, that is the products of six second-quantized operators. To effect the cancelation, the nonlinearity of the expansion coefficients of  $\hat{C}$  must be increased from  $b_j b_{klm}$  to  $b_j c_k d_l e_m$ . Specifically, the  $\hat{C}$  operators in Table I are defined as

$$\hat{C}_{uvwz} = \sum_{jklm} b_j^u c_k^v d_l^w e_m^z \hat{a}_j^u \hat{a}_k^v \hat{a}_l^w \hat{a}_m^z, \quad (26)$$

where  $\hat{a}_j^u$  and  $b_j^u$  are  $\hat{a}_j^{\dagger}$  and  $b_j^*$  if  $u = x$  and  $\hat{a}_j$  and  $b_j$  if  $u = o$ . Each of the eight (2,4)-positivity conditions in Table I generates an additional condition by switching all  $x$ 's and  $o$ 's in accordance with *particle-hole duality*, the symmetry between particles and holes. The (2,4)-conditions become the diagonal  $N$ -representability conditions [7, 32–34] when  $b$ ,  $c$ ,  $d$ , and  $e$  are restricted to be unit vectors; they are more general than the unitarily invariant diagonal conditions because these four vectors are not required to be orthogonal. These (2,4)-positivity conditions are only representative of the process by which complete conditions can be constructed from the solution of the  $N$ -representability problem presented in this

Letter. Additional (2,4)-conditions in this class can be generated from reordering creation and annihilation operators in the conditions of Table I, and other extreme (2,4)-conditions can be constructed from lifting the (2,3)-conditions. A comprehensive list of (2,4)-positivity conditions as well as (2,3)-, (2,5)-, and (2,6)-positivity conditions, which are consistent with the constructive solution, will be presented elsewhere [31]. The (2,5)- and (2,6)-conditions include extensions of three and eighteen classes of known diagonal conditions, respectively.

The set  $P_N^{2*}$  of  $N$ -representability conditions on the 2-RDM contains the set  $C_N^{2*}$  of *classical  $N$ -representability conditions* [7, 32–34], which ensure that the two-electron reduced density function (2-RDF), the diagonal (classical) part of the 2-RDM, can be represented by the integration of a  $N$ -particle density function. In different fields the set  $C_N^2$  of  $N$ -representable 2-RDF has been given different names: cut polytope [32] in combinatorial optimization and the correlation (or Boole) polytope [32, 36] in the study of 0-1 programming or Bell's inequalities. The set  $C_N^2$ , previously characterized, has important applications in global optimization including the search for the global energy minima of molecular clusters [34], the study of classical fluids [35], the max-cut problem in circuit design and spin glasses [32], lattice holes in the geometry of numbers, pair density (2-RDF) functional theory [33], and the investigation of generalized Bell's inequalities [36]. The characterization of the set  $P_N^2$  of  $N$ -representable 2-RDMs represents a significant generalization of the solution of the classical  $N$ -representability problem (the Boole 0-1 programming problem). In addition to its potentially significant applications to the study of correlation in many-fermion quantum systems, knowledge of the set  $P_N^2$  may have important applications to “quantum” analogues of problems in circuit design and the geometry of numbers.

The complete set of  $N$ -representability conditions firmly solidifies 2-RDM theory as a fundamental theory of many-body quantum mechanics with two-particle interactions. Rigorous lower bounds to the ground-state energy of strongly correlated quantum systems can be computed and improved in polynomial time from sub-

sets of the complete  $N$ -representability conditions [20] (Minimizing the energy with a fully  $N$ -representable 2-RDM is a non-deterministic polynomial (NP) complete problem because  $C_N^2 \subset P_N^2$  with optimization in  $C_N^2$  known to be NP-complete [32]). The present result raises challenges and opportunities for future research that include (i) implementing the higher  $N$ -representability conditions which are not in the form of traditional semidefinite programming [14, 15, 20], and (ii) determining which of the new conditions are most appropriate for different problems in many-particle chemistry and physics. Beyond their potential computational applications, the complete  $N$ -representability conditions for fermionic density matrices provide new fundamental insight into many-electron quantum mechanics including the identification and measurement of correlation and entanglement.

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